SANDIA NATIONAL LABORATORIES
QUALITY ASSURANCE PROGRAM
for the
OFFICE of CIVILIAN RADIOACTIVE WASTE MANAGEMENT

QAP 20-2

SCIENTIFIC NOTEBOOKS
and
ROUTINE CALCULATIONS

Revision 1

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CHANGE HISTORY

Revision	Description	Effective Date
0	This is the initial version of this document.	05/11/2004
1	Administrative changes resulting from Audit OQA-FS-04-07	05/20/2004

TABLE OF CONTENTS

1.0 Purpose and Scope

This procedure prescribes requirements for the preparation and use of a Scientific Notebook (SN) to document OSTI scientific investigations, or other OSTI associated activities where this format would facilitate recording information.

Scientific Notebooks are intended to be used to record information characterized by new research, data collection, prototyping, new methodologies, or other non-routine activities typically conducted in laboratories, field activities analysis, routine calculations, or field activities.

Acronyms and definitions for terms used in this procedure may be found in the OSTI Glossary.

2.0 Implementation Actions

2.1 Initiation of Scientific Notebooks

Notebooks are obtained from the Notebook Coordinator, numbered, titled and entered in the Notebook Log.

The principal investigator (PI) determines when a SN is to be used, and references the SN in the appropriate Test Plan in accordance with QAP 20-1, Planning Documents. The information recorded in an SN should be related, i.e., a single SN should not be used for recording information from different investigations, analyses, projects, etc. A notebook may relate to a single task identified in the TP.

2.2 General Requirements for Scientific Notebooks

Scientific Notebooks shall contain:

- A reference to the planning document(s) and tasks identified in the plans to be covered by the notebook documentation;
- A statement of the objectives and description of work to be performed, or reference to an approved planning document or implementing document that describes the work;
- Identification of the method(s) used;
- The review schedule established for the notebook;
- Identification of the computer programs used (name, version, platform);
- Identification of manufacturer name, lot number, expiration date, if applicable, of chemicals used to prepare samples, and any specific non-standard handling control and maintenance;
- Identification of equipment and samples used;
- Identification of measuring and test equipment used and a reference to any corrective action/nonconformance generated in accordance with QAP16-1;
- A description of the work performed and the results obtained;
- The names of individuals performing the work;
- Dated initials or signature of individuals making the entries to identify the author, particularly when more than one individual makes entries;
- A description of changes made to methods used;

- A description of the potential sources of uncertainty and error in test plans, procedures, calculations, and parameters that must be controlled and measured to assure that tests are valid.

A Standard for OSTI Scientific Notebooks is given in Appendix A.

2.3 Routine Calculations

Routine calculations associated with TPs are to be documented in SNs and associated referenced supplementary documents.

2.3.1 Documentation of Routine Calculations

Documentation for routine calculations shall follow the criteria in Appendix B.

Note: Routine calculations normally stand-alone; however, several routine calculations may be conducted under a Test Plan for analyses. In the latter case, the routine calculations can be reviewed as part of the analysis records and do not require a separate review as described above. When computer software applications are changed or developed these shall comply with requirements of QAP 19-1.

2.4 Technical Reviews of Scientific Notebooks

An independent, technically qualified individual to verify technical adequacy and to ensure there is sufficient detail to shall review scientific Notebooks periodically:

- Retrace the investigations and confirm the results and calculations or
- Repeat the investigation and achieve comparable results without recourse to the original investigator.

Scientific Notebooks shall be reviewed:

- After the initial planning entries are made. At a minimum these included the firs four items listed in section 2.2 and other information the PI believes is needed to establish the experimental process
- Annually
- As requested by the PI or Manager
- Closure

Supplementary or supporting information in binders or other formats shall receive the same review cycle as the governing SN.

The technical reviewer shall document that the review was performed and what part(s) of the notebook were reviewed by signing and dating the SN in an appropriate location, or by documenting the review on a Document Review and Comment (DRC) form, Form QAP 6-1-1. Routine calculations if recorded in a scientific notebook or made separately shall receive both technical and QA review and approval.

The technical review of calculation shall be accomplished using one of the following methods:

- Separate independent calculations of the original work
- A check of the steps in the original calculations
- A spot or random check of the original calculations.

The technical reviewer shall document the choice of the method used, along with his/her name and signature, the date of the review, and the results of the review.

The QA reviewer shall document the results of the review, and the compliance with OSTI procedures, and provide his/her name, signature, and the date of the review.

Both technical and QA review can be documented on Form QAP 6-1-1, Document Review and Comment Form (DRC), or directly on the document itself. DRCs must be submitted to the OSTI Records Center with the calculation, spreadsheet, or listing of the auxiliary/utility code. Non-Routine Calculation conform to the Appropriate TP and are subject to data review and approval.

2.5 Closure of Scientific Notebooks

The PI is responsible for submitting the completed SN to the Records Center. The final SN entry shall be immediately followed by the printed names and dated signatures of both the PI and the technical reviewer.

3.0 Records

The following QA records, generated through implementation of this procedure, shall be prepared and submitted to OCRWM and a copy to the SNL Records Center in accordance with QAP 17-1 (Records):

QA Record

- Scientific Notebook and supporting documentation
- Completed Document Review and Comment

4.0 Appendices

Appendix A: Standard for OSTI Scientific Notebooks
Appendix B: Routine Calculations

Appendix A

OSTI Scientific Notebook Standard

Scientific Notebooks (SNs) create a permanent record which provides sufficient information for an independent person with equivalent technical background to understand the work, evaluate the technical quality of the work, continue unfinished work, and reproduce the work and its primary results. This Standard of Excellence is provided to improve the quality and consistency of these notebooks.

INTRODUCTION: This part of the SN describes the contents of the SN. It documents technical planning for the subject activity, and describes how specific QA requirements are implemented. The following information should be included:

- Work activity title.
- Unique scientific notebook identifying number.
- Initiation date.
- Principal investigator(s) - notebook owner's name(s).
- Table of Contents.
- List of authorized users (if more than one individual will be making entries into the notebook).
- A sample of each user's signature and initials (documented in the front of the notebook).
- Frequency of QA and technical reviews, and who will perform them.
- Clear statement of work objectives.
- Summary description of the work process.

BODY: This part of the SN contains the technical data. The organization of this section should be tailored to the particular activity. For example, it could be broken into subsections containing data from a series of experiments, a group of measurements, or a series of chronological observations. Each section should be clearly delineated with a tab/introductory page. The following information should be included in the body of the SN as appropriate:

- Description of the experimental or measurement system and process,
- Identification of samples collected or used,
- Identification of chemicals used, including name, manufacturer name, lot number, and expiration date if applicable,
- Description of required environmental conditions,
- Pertinent equipment calibration information,
- Listing or reference to data supplied by others,
- Identification of software and hardware used, related verification information.

CLOSEOUT: This part of the SN should contain a brief wrap-up statement summarizing results, where the information will be used or reported, and the dated signatures of the principal investigator(s) and final technical reviewer. If appropriate, a more detailed summary of results and reference(s) to related reports or papers may be included.

Format: The preferred format for SNs is a bound notebook with consecutively numbered pages.

The Principal Investigator (PI) who is the notebook owner determines the format, since some activities may require a ring-binder notebook to allow incorporation of computer output

or alternative media i.e., photographs, digital images, or magnetic media. Ring-binder notebooks may also be desirable if the work requires multiple subsections for parallel activities. Any auxiliary notebooks or binders are to be referenced in the notebook and the binders are to reference both the notebook and planning document(s). If parallel subsections are used, each section should be clearly delineated in the table of contents, and pages numbered with a unique section identifier and sequential page number (e.g., A-1, A-2...). If alternative media are attached to notebook pages, they must be attached in a fashion that assures long-term durability. If alternative media are of a form that cannot be readily incorporated into the notebook, they may be saved as separate records with appropriate identification numbers and associated pointers in the SN.

Entries: All entries/additions to a scientific notebook should be permanent. Black ink is preferred.

Some activities may require black lead or colored pencils, as in geologic mapping or core logging. If removal or exchange of materials is warranted (e.g., a data printout that includes additional columns or new data), an explanation should be included as either a log in the introductory section, or as a notation in the body of the notebook.

Examples of types of information to be entered in the SN include: raw data; model numbers, serial numbers, and calibration certification dates of standards used; instrument calibration results; problems encountered; test results; printout copies of results; data reduction steps performed i.e., outlier testing, averaging, statistical analysis. Software information (including hardware, platform etc.), macros/routines, equations shall also be entered into the notebook. When notebooks are used to document calculations or analysis, the documentation is to comply with Appendix B Routine Calculations and requirements of The TP Traceability of data, calibration activities and calibration standards is critical (traceability from raw data to spread sheets to reduction/analysis files by referencing complete filenames).

Corrections to SN entries shall be made in accordance with QAP 17-1 (Records).

If the correction or change is substantial, an explanation should be provided. If there is a fundamental change in the approach or strategy of the work, a detailed explanation should be recorded.

Blank Pages: Areas or pages that are left blank should have a line drawn diagonally through the blank area, with the dated initials of the individual who drew the line.

Handling and Storage: Handling and Storage of a scientific notebook are the responsibility of the notebook owner.

Protection of a scientific notebook is important, since it often is the only documentation of ongoing work. When not in direct use, notebooks should be stored in a secure, fire resistant area. Periodically (frequency determined by the PI) the information in the SN should be protected from loss by copying the information, and storing the copy at a separate, remote location.

Technical Review: An independent technical review is the best way to review the technical content of the SN, and examine the notebook from the perspective of replicating the work.

The introductory section of the SN should specify the frequency of reviews (periodic or on completion of specific work segments), who will review the SN, and how reviews will be recorded in the notebook, i.e., on a review sheet in the introductory section, or within specific notebook subsections.

Quality Assurance Reviews: QA reviews of the SN should be conducted periodically and prior to submission of the SN to OCRWM and a copy to the SNL Records Center to assure appropriate QA requirements and process controls have been implemented.

Appendix B

Routine Calculation Requirements

Documentation of routine calculations is intended to provide sufficient detail to allow reproducibility of the calculation, spreadsheet, or auxiliary/utility code by an independent technical person. Documentation of routine calculations can be in any format (e.g., memo, scientific notebook, contractor report). The author (e.g., Principal Investigator, analyst, designee) shall ensure the following information is included:

1. Title of calculation

2. Associated planning document identifier (e.g., analysis plan, test plan), if applicable

3. A clear description of each step or clear definition of each algorithm used in the calculation, spreadsheet, or auxiliary/utility code.

4. Identification/listing of input, input sources, and output

5. Data qualification or justification:

6. If software was used to do the calculation (e.g., a spreadsheet, database, or graphing program), identify the name and version of the software, the platform on which it was run, and illustrate how the specific application provides the correct results for the specified range of input parameters.

   Note: The software used for routine calculations should be submitted as part of the documentation if needed for reproducibility.

7. Dates and results of reviews, along with the names and signatures of the analyst and reviewers (technical and QA.)